Orthogonalization of correlated states

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A scheme for orthogonalizing correlated states while preserving the diagonal matrix elements of the Hamiltonian is developed. Conventional perturbation theory can be used with the orthonormal correlated basis obtained from this scheme. Advantages of using orthonormal correlated states in calculations of the response function and correlation energy are discussed.

I. INTRODUCTION

Correlated basis theories[1,2] of Fermi liquids are a natural extension of the variational theories in which the trial ground state is written as

$$|0)=\frac{G|0]}{[0|G^{\dagger}G|0]^{1/2}}\ , \tag{1.1}$$

where $|0]$ is the ground state of ideal Fermi gas, and G is a suitably chosen correlation operator. We use $|\ ]$ and $|\ )$ to denote noninteracting and correlated states, respectively. In the early days of these theories G was taken as a product of Jastrow pair correlation functions

$$G=\prod_{i<j} f(r_{ij})\ , \tag{1.2}$$

and the $f(r_{ij})$ was determined by minimizing the ground state energy

$$E_0=(0|H|0)\ . \tag{1.3}$$

In more recent work[3-6] correlation operators containing two-body backflow or spin correlations, as well as three-body correlations have been used.

The correlated basis (CB) states are defined as

$$|\mathbf{p}_1\cdots\mathbf{p}_n\mathbf{h}_1\cdots\mathbf{h}_n)\equiv\frac{G|\mathbf{p}_1\cdots\mathbf{p}_n\mathbf{h}_1\cdots\mathbf{h}_n]}{[\mathbf{p}_1\cdots\mathbf{p}_n\mathbf{h}_1\cdots\mathbf{h}_n|G^{\dagger}G|\mathbf{p}_1\cdots\mathbf{p}_n\mathbf{h}_1\cdots\mathbf{h}_n]^{1/2}}\ , \tag{1.4}$$

where $|\mathbf{p}_1\cdots\mathbf{p}_n\mathbf{h}_1\cdots\mathbf{h}_n]$ is the n-particle n-hole Fermi gas state, and $|\mathbf{p}_1\cdots\mathbf{h}_n)$ is the corresponding n-particle n-hole CB state. The CB states are normalized but not orthogonal to each other. They have been used with nonorthogonal basis perturbation theory[7] to study various properties of quantum liquids. This approach, which is often called CBPT (correlated-basis perturbation theory), has been proved to be renormalizable and the perturbative series corresponding to the energy eigenvalues have been explicitly derived.[8] Recently, detailed microscopic calculations on helium liquids[9-11] and nuclear matter[12,13] have been performed by using the low order CBPT theory.

A clear analysis of the convergence properties of the CBPT theory has not yet been done and, in particular, the truncation of the series at some perturbative order generally leads to nonorthogonality spuriosities whose effects may not be negligible. Moreover, the properly orthogonalized eigenvectors cannot be easily extracted out from CBPT and this may be a major problem in calculating quantities other than the eigenvalues of the Hamiltonian.

In studies of hot quantum liquids the free-energy $F(\rho,T)$ obtained with CB states has been minimized. The results obtained for the $F(\rho,T)$ of ^{3}He liquid[14] and nuclear matter[15] are reasonable, but the corrections due to nonorthogonality have not been calculated. If the states are orthogonal, the calculated $F(\rho,T)$ is an upper bound due to the variational principle. It is interesting to inquire if this variational property remains when the nonorthogonal CB states are used.

The dynamical structure function $S(k,\omega)$ of nuclear matter, calculated with the nonorthogonalized 1p-1h CB states does not satisfy the sum rule

$$\int S(k,\omega)d\omega=S(k)\ . \tag{1.5}$$

The static structure function $S(k)$ obtained from 1p-1h CB states has the wrong behavior at $k\rightarrow\infty$ because of the spuriosity due to the lack of orthogonality amongst the 1p-1h CB states.[16]

It is possible to orthogonalize a set of states by using the Löwdin[17] transformation. However, it is known that if all CB states are orthogonalized together the resulting orthogonal states are not as good as the CB states in several respects. For instance, the expectation value of the Hamiltonian in the ground state of the orthogonalized set is higher than E_0 of the CB ground state,[1,18] whereas the ground state eigenvalue must be below E_0 by the variational principle. Therefore, the two-step process, in which the CB states are first orthogonalized by using the Löwdin transformations and then used in per-

turbations theory, is not recommended. The Löwdin orthogonalization moves up the energies of low lying states, and the perturbative corrections move them down, both effects being larger than the net displacement.[1,18] In nonorthogonal basis theory only the net displacement is calculated.

In this paper we propose an orthogonal correlated basis (OCB) theory in which we first orthogonalize the CB states and then use them in perturbation theory. The problems mentioned above are avoided by using a combination of Schmidt and Löwdin orthogonalizations such that the energies of the orthogonal states are equal to those of CB states in the thermodynamic limit. Therefore, conventional perturbation theory with these states has a convergence at least as good as that of the nonorthogonal basis theory.

The general properties of the CB matrix elements of the unit and the Hamiltonian operators are reviewed in Sec. II. Most of the material in this section is not new; however, our objectives are different from those of the earlier works. It is primarily reviewed for the sake of completeness and to clarify the notation. The properties of the matrix elements with the new states are given in Sec. III. Section IV is devoted to the discussion of the proposed OCB theory in the case of two examples of interest, the dynamical structure function and the perturbative correction to the variational ground state energy E_0.

II. CB MATRIX ELEMENTS

In this section we review the calculation and the properties of the matrix elements $(\mathbf{p}_1' \cdots \mathbf{h}_m' \mid \mathbf{p}_1 \cdots \mathbf{h}_n)$ and $(\mathbf{p}_1' \cdots \mathbf{h}_m' \mid H \mid \mathbf{p}_1 \cdots \mathbf{h}_n)$ using well known diagrammatic methods.[1-3,19] These properties are used in Sec. III to construct the desired orthogonal set. The CB matrix elements are constructed from the Fermi-gas (FG) matrix elements

$$[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] ,$$

and

$$[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid G^\dagger H G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] . \tag{2.1}$$

The FG matrix elements are expanded by substituting

$$\begin{aligned} G &= \prod_{i<j} f_{ij} \prod_{i<j<k} f_{ijk} \\ &= \prod_{i<j} (1+F_{ij}) \prod_{i<j<k} (1+F_{ijk}) , \end{aligned} \tag{2.2}$$

where $F_{ij} \equiv f_{ij} - 1$ and $F_{ijk} \equiv f_{ijk} - 1$ are functions of short range. They then break up into a sum over integrals that contain small groups (clusters) of particles. The terms of this expansion are represented by diagrams using the following notation.

The points or vertices of the diagrams represent coordinates $\mathbf{r}_i$ to be integrated, and correlation lines represent the functions $f_{ij}^\dagger f_{ij} - 1$, $f_{ijk}^\dagger f_{ijk} - 1$, etc., in the integral. We use dashed lines to denote these functions. A factor $\exp[i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]$ is obtained when the state $\mathbf{k}$ is occupied in the bra $[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid$ by a particle j, and in the ket $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$ by a particle i. This factor is denoted by a line that starts from vertex i, ends on vertex j, and has a direction arrow labeled $\mathbf{k}$. These lines are called state (or exchange) lines.

Diagrams representing terms in the expansion of the diagonal matrix element $[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n]$ can have a number of points $\mathbf{r}_1, \mathbf{r}_2, \ldots$, connected by either correlation or exchange lines. All points may form a single connected piece or two or more disconnected pieces as illustrated in Figs. 1(a) and (b). In principle all diagrams should have N points, where N is the number of particles in the liquid. However, isolated unconnected points, as in diagram (c) of Fig. 1, are not shown because they give unit factor. Diagrams in which uncorrelated particles are exchanged, such as shown in Fig. 1(d) are discarded because they give zero contribution. The exchange lines must form closed loops, and can have momenta of states occupied in $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$. The contribution of a diagram is given by

$$\frac{1}{s} \frac{1}{\Omega^{N_k}} (-1)^{N_k - N_l} \int \prod_{i=1,N_k} d^3 r_i$$

(product of all correlation and exchange lines) . (2.3)

Here Ω is the normalization volume, and we assume the thermodynamic limit in which N and $\Omega \to \infty$ at fixed density $\rho = N/\Omega$. N_k is the number of state lines in the diagram; it also equals the number of vertices in the diagram by construction. The factor Ω^{-N_k} takes into account the normalization of the plane wave states. N_l is the number of closed loops, and $(-1)^{N_k - N_l}$ takes into account the sign changes due to exchange. Only one way of labeling the particles in the diagrams is considered, i.e., all diagrams that can be obtained by labeling the points 1, 2, 3, and 4 in diagram a of of Fig. 1 in a different way are ignored. If we keep all the N points in the diagram, then there are $N!/s$ ways of labeling them, where the symmetry factor s equals the number of exchanges which leave

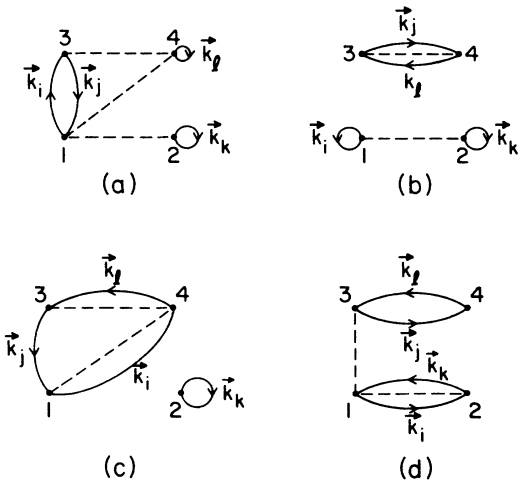

FIG. 1. Examples of cluster diagrams in the expansion of $[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n]$.

the diagram unchanged. The $N!$ factor is used to cancel the two $1/\sqrt{N!}$ factors in the normalization of the Fermi-gas states.

In principle all diagrams that come from expanding $[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n]$ have one state line for every momenta occupied in $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$. All the labels $\mathbf{k}_1, \mathbf{k}_2, \ldots,$ in a diagram, thus, must be different from each other; however, this restriction $\mathbf{k}_1 \neq \mathbf{k}_2 \neq \mathbf{k}_3 \ldots$, can be ignored because diagrams with two or more identical state lines cancel each other as illustrated in Fig. 2.

A. CB matrix elements of the identity operator

We first calculate the ratio of normalizations

$$\frac{[\mathbf{p}_1 \ldots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \ldots \mathbf{h}_n]}{[\mathbf{p}_1' \ldots \mathbf{h}_m' \mid G^\dagger G \mid \mathbf{p}_1' \ldots \mathbf{h}_m']}, \tag{2.4}$$

which occurs in many expressions. Let $\mathbf{c}_1, \mathbf{c}_2 \ldots$, be the single-particle states occupied in both kets $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$ and $\mid \mathbf{p}_1' \cdots \mathbf{h}_m']$; $\mathbf{a}_1, \mathbf{a}_2 \cdots \mathbf{a}_D$ be the D states that are occupied in $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$ but not in $\mid \mathbf{p}_1' \cdots \mathbf{h}_m']$, and $\mathbf{b}_1, \mathbf{b}_2 \cdots \mathbf{b}_D$ are occupied in $\mid \mathbf{p}_1' \cdots \mathbf{h}_m']$ but not in $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$. We assume that the number of states $\mathbf{c}_i$ is proportional to Ω, but D is finite. The nondiagonal matrix elements of the unit and Hamiltonian operators between two states that differ in D orbits would be practically zero when D is large.

The numerator of (2.4) can be written as

$$[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] = \left[1 + \Sigma_1(\mathbf{a}_1, \mathbf{a}_2 \cdots \mathbf{a}_D)\right] \times \left[1 + \Sigma_A(\mathbf{c}_i \text{ only})\right], \tag{2.5}$$

where $\Sigma_1(\mathbf{a}_1, \mathbf{a}_2 \cdots \mathbf{a}_D)$ is the sum of diagrams which contain one or more of the lines $\mathbf{a}_1 \cdots \mathbf{a}_D$ and any number of $\mathbf{c}_i$ lines, and in which a line $\mathbf{a}_i$ occurs, at most, once, while a line $\mathbf{c}_i$ may occur any number of times. $\Sigma_A(\mathbf{c}_i \text{ only})$ is the sum of diagrams having only $\mathbf{c}_i$ lines; a line $\mathbf{c}_i$ can occur any number of times. We can further simplify (2.5) as follows:

$$\Sigma_1(\mathbf{a}_1, \mathbf{a}_2 \cdots \mathbf{a}_D) = \sum_{i=1,D} \Sigma_c(\mathbf{a}_i) + \sum_{i=1,D} \sum_{j<i} \left[\Sigma_c(\mathbf{a}_i)\Sigma_c(\mathbf{a}_j) + \Sigma_c(\mathbf{a}_i + \mathbf{a}_j)\right] + \cdots, \tag{2.6}$$

where $\Sigma_c(\mathbf{a}_i)$ is the sum of connected diagrams having one $\mathbf{a}_i$ line and any number of $\mathbf{c}_i$ lines, while $\Sigma_c(\mathbf{a}_i + \mathbf{a}_j)$ is the sum of connected diagrams having one $\mathbf{a}_i$ and one $\mathbf{a}_j$ line, etc. A generic diagram contributing to $\Sigma_c(\mathbf{a}_i)$ has N_k points and $N_k - 1$ $\mathbf{c}_i$ lines, and its contribution is of the order of Ω^{-N_k+1} from Eq. (2.3). Note that since all correlations and state lines are functions of interparticle distances we obtain a factor Ω for every connected piece in the diagram from the integrations over $\mathbf{r}_i$. The sum over $N_k - 1$ $\mathbf{c}_i$'s gives a factor Ω^{N_k-1}, and hence $\Sigma_c(\mathbf{a}_i)$ is of order 1. On the other hand, $\Sigma_c(\mathbf{a}_i + \mathbf{a}_j)$ diagrams are also of order Ω^{-N_k+1} before summing over the $\mathbf{c}_i$; however, they have $N_k - 2$ $\mathbf{c}_i$ lines, and so the sum over $\mathbf{c}_i$ gives a factor Ω^{N_k-2}. Thus, $\Sigma_c(\mathbf{a}_i + \mathbf{a}_j)$ is of order Ω^{-1}, $\Sigma_c(\mathbf{a}_i + \mathbf{a}_j + \mathbf{a}_k)$ is of order Ω^{-2}, etc. We neglect them in the limit $\Omega \to \infty$ and obtain

$$[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] = \left[1 + \Sigma_A(\mathbf{c}_i \text{ only})\right] \times \prod_{i=1,D} \left[1 + \Sigma_c(\mathbf{a}_i)\right]. \tag{2.7}$$

A similar expression can be obtained for the denominator of (2.4), and

$$\frac{[\mathbf{p}_1 \cdots \mathbf{h}_n \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n]}{[\mathbf{p}_i' \cdots \mathbf{h}_m' \mid G^\dagger G \mid \mathbf{p}_1' \cdots \mathbf{h}_m']} = \prod_{i=1,D} \frac{\left[1 + \Sigma_c(\mathbf{a}_i)\right]}{\left[1 + \Sigma_c(\mathbf{b}_i)\right]}. \tag{2.8}$$

When G contains only Jastrow correlations, $\Sigma_c(a_i)$ can be further simplified to obtain a sum of only irreducible diagrams.[19]

Nondiagonal CB matrix elements of the identity operators are, in general, different from zero, since CB states are not orthogonal. The diagrams occurring in the expansion of

$$[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] \tag{2.9}$$

have D transition lines going from vertex i to j with two arrows and two labels $\mathbf{a}_k$ and $\mathbf{b}_k'$. These indicate that particle i was in state $\mathbf{a}_k$ in the ket $\mid \mathbf{p}_1 \cdots \mathbf{h}_n]$, and j in state $\mathbf{b}_k'$ in the bra $[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid$. The pairs $\mathbf{a}_k \mathbf{b}_k'$ can be chosen at convenience; however, diagrams such as (b) and (c) or (d) and (e) of Fig. 3, which differ only in the choice of the pairs $\mathbf{a}_k \mathbf{b}_k'$ are in fact identical and only one choice of pairs $\mathbf{a}_k \mathbf{b}_k'$ should be considered. One obtains

$$[\mathbf{p}_1' \cdots \mathbf{h}_m' \mid G^\dagger G \mid \mathbf{p}_1 \cdots \mathbf{h}_n] = \left[\Sigma_1(\mathbf{a}_1\mathbf{b}_1 + \mathbf{a}_2\mathbf{b}_2 + \cdots + \mathbf{a}_D\mathbf{b}_D)\right] \times \left[1 + \Sigma_A(c_i \text{ only})\right], \tag{2.10}$$

where $\Sigma_1(\mathbf{a}_1\mathbf{b}_1 + \mathbf{a}_2\mathbf{b}_2 + \cdots + \mathbf{a}_D\mathbf{b}_D)$ is the sum of diagrams containing one each of the D transition lines and any number of $\mathbf{c}_i$ lines. The CB matrix element is given by

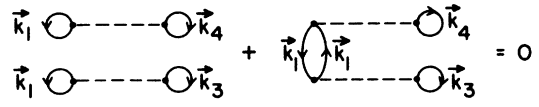

FIG. 2. Cancellation of diagrams with more than one k_1 line.

$$(\mathbf{p}'_1\cdots\mathbf{h}'_m\mid\mathbf{p}_1\cdots\mathbf{h}_n)=\frac{[\mathbf{p}'_1\cdots\mathbf{h}'_m\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]}{[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]}\left[\frac{[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]}{[\mathbf{p}'_1\cdots\mathbf{h}'_m\mid G^\dagger G\mid\mathbf{p}'_1\cdots\mathbf{h}'_m]}\right]^{1/2}$$

$$=\frac{\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\mathbf{a}_2\mathbf{b}_2+\cdots+\mathbf{a}_D\mathbf{b}_D)}{\prod_{i=1,D}\left[1+\Sigma_c(\mathbf{a}_i)\right]^{1/2}\left[1+\Sigma_c(\mathbf{b}_i)\right]^{1/2}}\ . \tag{2.11}$$

Momentum conservation requires that

$$\sum_{i=1,D}\mathbf{a}_i=\sum_{i=1,D}\mathbf{b}_i\ . \tag{2.12}$$

If there are no subsets containing a number d of $\mathbf{a}_i$'s and $\mathbf{b}_i$'s, $d<D$, such that

$$\sum_{i\text{ in }d}\mathbf{a}_i=\sum_{i\text{ in }d}\mathbf{b}_i\ , \tag{2.13}$$

all the transition lines must occur in a single connected diagram, and the order of magnitude of the matrix element (2.11) is Ω^{-D+1}. We note that, since momentum conservation requires a change in at least two states, $D\geq 2$. Let S be the number of subsets satisfying Eq. (2.13), $S=1$ if there are no such subsets. Since each subset must have changes in two or more momentum states, $2S<D$. If $S\geq 2$ we can have disconnected diagrams, as illustrated in Fig. 4(b), contributing to the numerator of (2.11). In this case (2.11) is of order Ω^{-D+2}. In general order of magnitude of

$$(\mathbf{p}'_1\cdots\mathbf{h}'_m\mid\mathbf{p}_1\cdots\mathbf{h}_n)=\Omega^{-D+S}\ , \tag{2.14}$$

$$D\geq 2S\ , \tag{2.15}$$

$$S\geq 1\ . \tag{2.16}$$

B. CB matrix elements of the Hamiltonian

Let us consider diagonal CB matrix elements of the Hamiltonian:

$$H=-\sum_{i=1,N}\frac{\hbar^2}{2m}\nabla_i^2+\sum_{i<j\leq N}v_{ij}+\sum_{i<j<k\leq N}V_{ijk}+\cdots\ . \tag{2.17}$$

The terms in $[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger HG\mid\mathbf{p}_1\cdots\mathbf{h}_n]$ in which the ∇_i^2 operate on the ket $\mid\mathbf{p}_1\cdots\mathbf{h}_n]$ give

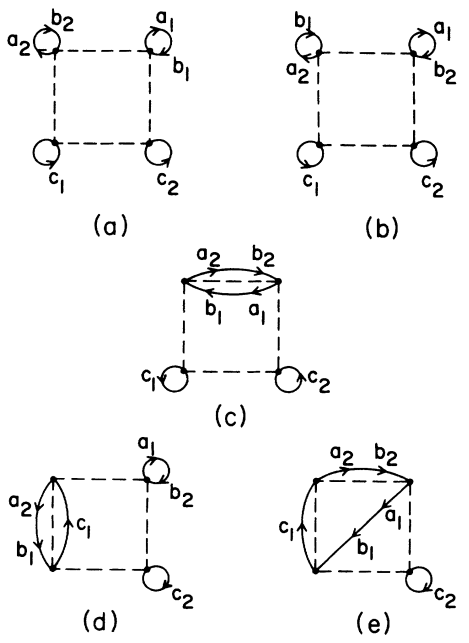

FIG. 3. Examples of cluster diagrams in the expansion of $[\mathbf{p}'_1\cdots\mathbf{h}'_m\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]$.

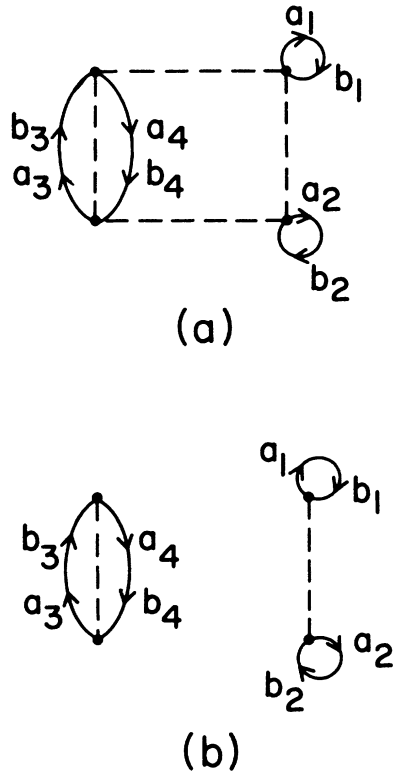

FIG. 4. Connected and disconnected diagrams in the expansion of $[\mathbf{p}'_1\cdots\mathbf{h}'_m\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]$.

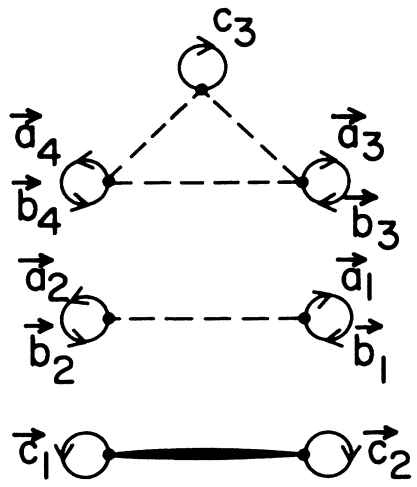

FIG. 5. Example of disconnected diagrams in the expansion $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)$.

$$T_F(\mathbf{p}_1\cdots\mathbf{h}_n)[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]\,, \tag{2.18}$$

$$T_F(\mathbf{p}_1\cdots\mathbf{h}_n)=\sum_{i=1,N}\frac{\hbar^2}{2m}k_i^2\,. \tag{2.19}$$

We denote all the states occupied in $\mid\mathbf{p}_1\cdots\mathbf{h}_n]$ by $\mathbf{k}_i$, $i=1,N$. Thus $\mathbf{k}_i$, $i=1,N$ is the sum of the states $\mathbf{c}_i$, $i=1$, $N-D$ and $\mathbf{a}_i$, $i=1,D$. The other terms of $[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger HG\mid\mathbf{p}_1\cdots\mathbf{h}_n]$ contain either one of the potentials v_{ij}, V_{ijk}, etc., or gradients of correlations $\nabla_i^2 f_{ij}$, $\nabla_i f_{ij}\cdot\nabla_i f_{ik}$, $\nabla_i f_{ij}\cdot\nabla_i\mid\mathbf{p}_1\cdots\mathbf{h}_n]$, etc., and they are evaluated with cluster expansions. In the diagramatic notation the functions $f_{ij}v_{ij}f_{ij}$, $f_{ij}\nabla^2 f_{ij}$, $f_{ij}f_{jk}\nabla_j f_{ij}\nabla_j f_{jk}$, $f_{ij}\nabla f_{ij}\cdot\nabla$, etc. are represented by interaction lines, and it is easy to show that

$$[\mathbf{p}_1\cdots\mathbf{h}_n\mid G^\dagger HG\mid\mathbf{p}_1\cdots\mathbf{h}_n]=\left[T_F(\mathbf{p}_1\cdots\mathbf{h}_n)+\Sigma_c(I)\right]\times\left[1+\Sigma_A(k_i\text{ only})\right]\,, \tag{2.20}$$

where $\Sigma_c(I)$ is the sum of all connected diagrams that have one interaction line and any number of lines $\mathbf{k}_i$, $i=1,N$. The diagonal CB matrix elements are given by

$$(\mathbf{p}_1\cdots\mathbf{h}_n\mid H\mid\mathbf{p}_1\cdots\mathbf{h}_n)=\Sigma_c(I)+T_F(\mathbf{p}_1\cdots\mathbf{h}_n)\,, \tag{2.21}$$

and are of order Ω.

The nondiagonal element

$$[\mathbf{p}_1'\cdots\mathbf{h}_m'\mid G^\dagger HG\mid\mathbf{p}_1\cdots\mathbf{h}_n]$$

has one term containing $T_F(\mathbf{p}_1\cdots\mathbf{h}_n)$ and others containing an interaction line. It can be expressed as

$$[\mathbf{p}_1'\cdots\mathbf{h}_m'\mid G^\dagger HG\mid\mathbf{p}_1\cdots\mathbf{h}_n]=T_F(\mathbf{p}_1\cdots\mathbf{h}_n)[\mathbf{p}_1'\cdots\mathbf{h}_m'\mid G^\dagger G\mid\mathbf{p}_1\cdots\mathbf{h}_n]+\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\mathbf{a}_2\mathbf{b}_2+\cdots\mathbf{a}_D\mathbf{b}_D+I)\left[1+\Sigma_A(\mathbf{c}_i\text{ only})\right]\,, \tag{2.22}$$

and we get

$$(\mathbf{p}_1'\cdots\mathbf{h}_m'\mid H\mid\mathbf{p}_1\cdots\mathbf{h}_n)=\frac{\left[T_F(\mathbf{p}_1\cdots\mathbf{h}_n)\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D)+\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)\right]}{\left\{\prod_{i=1,D}\left[1+\Sigma_c(\mathbf{a}_i)\right]^{1/2}\left[1+\Sigma_c(\mathbf{b}_i)\right]^{1/2}\right\}}\,. \tag{2.23}$$

If there are S subsets in the transition, the $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D)$ is of order Ω^{-D+S}, and the leading diagrams of $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)$ illustrated in Fig. 5, are of order Ω^{-D+S+1}. T_F is of order Ω, and, hence the order of magnitude of

$$(\mathbf{p}_1'\cdots\mathbf{h}_m'\mid H\mid\mathbf{p}_i\cdots\mathbf{h}_n)=\Omega^{-D+S+1}\,. \tag{2.24}$$

The largest terms have $D=2$, $S=1$ and they are of order 1.

The nonorthogonality of CB states raises the order of magnitude of the nondiagonal matrix elements of H by a factor Ω. Let us consider states near the CB ground state $\mid 0)$. These states have finite values of m and n. The matrix element

$$(\mathbf{p}_1'\cdots\mathbf{h}_m'\mid H-E_0\mid\mathbf{p}_1\cdots\mathbf{h}_n)$$

$$=\frac{\left\{\left[T_F(\mathbf{p}_1\cdots\mathbf{h}_n)-T_F(0)-\Sigma_c^0(I)\right]\Sigma_1(\mathbf{a}_1\mathbf{b}_1'+\cdots\mathbf{a}_D\mathbf{b}_D)+\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)\right\}}{\left\{\prod_{i=1,D}\left[1+\Sigma_c(\mathbf{a}_i)\right]^{1/2}\left[1+\Sigma_c(\mathbf{b}_i)\right]^{1/2}\right\}}\,, \tag{2.25}$$

where $\Sigma_c^0(I)$ is the sum of connected diagrams contributing to E_0. Now

$$T_F(\mathbf{p}_1\cdots\mathbf{h}_n)-T_f(0)=\frac{\hbar^2}{2m}\sum_{j=1,n}(p_j^2-h_j^2) \tag{2.26}$$

is finite, and the leading term of $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)$, of the type illustrated in Fig. 5 is separated out to obtain

$$\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)=\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D)\,\Sigma_c(I,\mathbf{c}_i\text{ only})+\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+\text{connected }I)\,, \tag{2.27}$$

where $\Sigma_c(I,\mathbf{c}_i$ only) is the sum of connected diagrams with an interaction line and any number of c_i lines, while $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+$connected $I)$ is the subset of $\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+I)$ diagrams in which the I line occurs together with a transition line in a connected diagram. The states $\mathbf{c}_i$ and those occupied in $|0]$ can be classified as a large (of order Ω) number of common states $\mathbf{z}_i$, states $\mathbf{x}_i$ that occur in $\mathbf{c}_i$ only, and states $\mathbf{y}_i$ that occur in $|0]$ only. We then have

$$\Sigma_c(I,\mathbf{c}_i\text{ only})-\Sigma_c^0(I)=\sum_i\Sigma_c(I+\mathbf{x}_i)-\sum_i\Sigma_c(I+\mathbf{y}_i)+\text{ terms of order }1/\Omega\,. \tag{2.28}$$

Here $\Sigma_c(I+\mathbf{x}_i)$ denotes the subset of $\Sigma_c(I,\mathbf{c}_i$ only) that has one $\mathbf{x}_i$ line, while $\Sigma_c(I+\mathbf{y}_i)$ is the subset of $\Sigma_c^0(I)$ that has one $\mathbf{y}_i$ line. These terms are of order 1. We obtain

$$(\mathbf{p}_1'\cdots\mathbf{h}_m'\,|\,H-E_0\,|\,\mathbf{p}_1\cdots\mathbf{h}_n)=\left\{\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D)\left[\frac{\hbar^2}{2m}\sum_{j=1,n}(p_j^2-h_j^2)+\sum_i\Sigma_c(I+\mathbf{x}_i)-\sum_i\Sigma_c(I+\mathbf{y}_i)\right]\right.$$
$$\left.+\,\Sigma_1(\mathbf{a}_1\mathbf{b}_1+\cdots\mathbf{a}_D\mathbf{b}_D+\text{connected }I)\right\}\Big/\prod_i\left[1+\Sigma_c(\mathbf{a}_i)\right]^{1/2}\left[1+\Sigma_c(\mathbf{b}_i)\right]^{1/2}, \tag{2.29}$$

which is of order Ω^{-D+S} instead of (2.23) which is of order Ω^{-D+S+1}. We note that the CB matrix elements of H are larger than those of 1 by a factor Ω, while those of $H-E_0$ are of same order of magnitude when m and n are finite.

III. CORRELATED ORTHOGONAL (CO) STATES

An intermediate, partially orthogonal (PO) set of states, denoted by $|\,\mathbf{p}_1\cdots\mathbf{h}_n\}$ is defined as

$$|\,\mathbf{p}_1\cdots\mathbf{h}_n\}=|\,\mathbf{p}_1\cdots\mathbf{h}_n)-\sum_{m<n}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_m'}|\,\mathbf{p}_1'\cdots\mathbf{h}_m')(\mathbf{p}_1'\cdots\mathbf{h}_m'\,|\,\mathbf{p}_1\cdots\mathbf{h}_n)\,. \tag{3.1}$$

The PO n-particle n-hole (n-ph) states are obtained by orthogonalizing the CB n-ph states to all $m<n$ ph CB states with Schmidt procedure. Since the CB n-ph state is directly coupled to few states with $m<n$ ph, the PO states are not too different from CB states. As we will see, the diagonal matrix elements do not change in going from CB to PO states in the limit $\Omega\to\infty$, and thus the PO states are normalized.

A PO n-ph state is orthogonal to all PO $m\neq n$ ph states by construction, but not to other n-ph PO states. Complete orthogonalization is obtained by making separate Löwdin transformations to orthogonalize the n-ph states among themselves

$$|\,\mathbf{p}_1\cdots\mathbf{h}_n\rangle=|\,\mathbf{p}_1\cdots\mathbf{h}_n\}-\tfrac{1}{2}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_n'}|\,\mathbf{p}_1'\cdots\mathbf{h}_n'\}\overline{\{\mathbf{p}_1'\cdots\mathbf{h}_n'\,|\,\mathbf{p}_1\cdots\mathbf{h}_n\}}$$
$$+\tfrac{3}{8}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_n'}\sum_{\mathbf{p}_1''\cdots\mathbf{h}_n''}|\,\mathbf{p}_1''\cdots\mathbf{h}_n''\}\overline{\{\mathbf{p}_1''\cdots\mathbf{h}_n''\,|\,\mathbf{p}_1'\cdots\mathbf{h}_n'\}}\,\overline{\{\mathbf{p}_1'\cdots\mathbf{h}_n'\,|\,\mathbf{p}_1\cdots\mathbf{h}_n\}}+\cdots\,. \tag{3.2}$$

The $|\,\mathbf{p}_1\cdots\mathbf{h}_n\rangle$ are the desired correlated orthonormal (CO) states. The coefficients $1,-\frac{1}{2},+\frac{3}{8}\ldots$, of the terms in the Löwdin transformation are those that occur in the expansion of $(1+x)^{-1/2}$. The bar on any matrix element denotes that diagonal elements are to be omitted,

$$\overline{(a\,|\,b)}\equiv(a\,|\,b)(1-\delta_{ab})\,, \tag{3.3}$$

where $|\,a)$ and $|\,b)$ are two states in any basis.

We will first study the properties of the diagonal matrix elements with PO states:

$$\{\mathbf{p}_1\cdots\mathbf{h}_n\,|\,\mathbf{p}_1\cdots\mathbf{h}_n\}=1-T_1+T_2\,, \tag{3.4}$$

$$T_1=\sum_{m<n}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_m'}|\,(\mathbf{p}_1'\cdots\mathbf{h}_m'\,|\,\mathbf{p}_1\cdots\mathbf{h}_n)\,|^2\,, \tag{3.5}$$

$$T_2=\sum_{m<n}\sum_{m'<n}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_m'}\sum_{\mathbf{p}_1''\cdots\mathbf{h}_{m'}''}(\mathbf{p}_1\cdots\mathbf{h}_n\,|\,\mathbf{p}_1''\cdots\mathbf{h}_{m'}'')\times\overline{(\mathbf{p}_1''\cdots\mathbf{h}_{m'}''\,|\,\mathbf{p}_1'\cdots\mathbf{h}_m')}\times(\mathbf{p}_1'\cdots\mathbf{h}_m'\,|\,\mathbf{p}_1\cdots\mathbf{h}_n)\,. \tag{3.6}$$

Using the properties of the CB matrix elements we prove in the following that T_1 is of order Ω^{-2} and T_2 of order Ω^{-3}, and therefore that these terms are negligible, and hence the PO states have unit norm.

Consider the term T_1. Let there be D' states $\mathbf{p}'_1 \cdots \mathbf{h}'_m$ that do not occur in $\mathbf{p}_1 \cdots \mathbf{h}_n$. The total number of different orbits in the states $|\mathbf{p}'_1 \cdots \mathbf{h}'_m)$ and $|\mathbf{p}_1 \cdots \mathbf{h}_n)$ is then given by

$$D = D' + n - m \ . \tag{3.7}$$

Since $D \geq 2$, $D' \geq 1$ if $m = n-1$, otherwise $D' \geq 0$. The contribution of matrix elements with $S=1$ and $D' > 1$ to T_1 is of order

$$(\Omega^{-D+1})^2 \Omega^{D'-1} = \Omega^{-D-(n-m)+1} \leq \Omega^{-2} \ . \tag{3.8}$$

The factor $\Omega^{D'-1}$ in the above estimate comes from summing over D' momenta with one momentum conservation constraint. Contribution of the matrix elements having $S=1$, $D'=0$ and, hence, $n-m \geq 2$ is of order $\Omega^{-2D+2} \leq \Omega^{-2}$. These are the largest contributions to T_1.

When $S=2$ we have two possibilities. The first is that one subgroup contains all the D' states, and the other contains some or all of the $n-m$ states that change. In this case $n-m \geq 2$, and the order of magnitude of the contribution is $\Omega^{-D-(n-m)+3} \leq \Omega^{-3}$ since $D \geq 4$ when $S=2$. The second possibility is that one subgroup contains a part of the D' states, and the other contains the rest. In this case $n-m \geq 1$, but we sum over D' momenta with two contains, and, hence, the contribution is still $\leq \Omega^{-3}$. This proves that the leading contribution to T_1 is of order Ω^{-2}. By using a similar procedure one can prove that the leading contribution to T_2 is of order Ω^{-3} and it comes from states such that all the three matrix elements in Eq. (3.6) have $D=2$. We also find

$$\{\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n\} = (\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) + \text{terms of order } \Omega^{-1} \text{or smaller} \ , \tag{3.9}$$

and

$$\{\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, (H - E_0) \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n\} = (\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H - E_0 \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) + \text{terms of magnitude } \Omega^{-2} \text{or smaller} \ . \tag{3.10}$$

In either case the changes in diagonal matrix elements, on going from CB to PO basis, are negligible in the limit $\Omega \to \infty$.

Let us now consider the off diagonal matrix elements of n-ph PO states and compare them with the corresponding matrix elements of CB states

$$\{\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n\} = (\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) - T'_1 + T'_2 \ , \tag{3.11}$$

$$T'_1 = \sum_{m<n} \sum_{\mathbf{p}''_1 \cdots \mathbf{h}''_m} (\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}''_1 \cdots \mathbf{h}''_m)(\mathbf{p}''_1 \cdots \mathbf{h}''_m \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) \ , \tag{3.12}$$

$$T'_2 = \sum_{m<n} \sum_{\mathbf{p}''_1 \cdots \mathbf{h}''_m} \sum_{m'<n} \sum_{\mathbf{p}'''_1 \cdots \mathbf{h}'''_{n'}} (\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}'''_1 \cdots \mathbf{h}'''_{m'}) \overline{(\mathbf{p}'''_1 \cdots \mathbf{h}'''_{m'} \,|\, \mathbf{p}''_1 \cdots \mathbf{h}''_m)} (\mathbf{p}''_1 \cdots \mathbf{h}''_m \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) \ . \tag{3.13}$$

The $(\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n)$ is of order Ω^{-D+S} and when $S=1$, we represent it in Fig. 6(a) as a box with D particle or hole lines from $\mathbf{p}_1 \cdots \mathbf{h}_n$ below it and the new D particle or hole lines from $\mathbf{p}'_1 \cdots \mathbf{h}'_n$ above it. Figure 6(b) shows a term of T'_1 in which two particles and a hole of the D states combine into a one particle state. The matrix element $(\mathbf{p}''_1 \cdots \mathbf{h}''_m \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n)$ in Fig. 6(b) is of order Ω^{-1}, while $(\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}''_1 \cdots \mathbf{h}''_m)$ is of order Ω^{-D+2}, and the contribution is of order Ω^{-D+1} when $S=1$. There are also other terms, such as those shown in Fig. 6(c) in T'_1, and Fig. 6(d) in T'_2 with contributions of order Ω^{-D+S}, but none of order Ω^{-D+S+1}. Thus, we obtain the result that the off diagonal elements of the unit, H or $H - E_0$ operators between n-ph states may be different in CB and PO states, but they have the same order of magnitude.

Finally, we prove that the diagonal matrix elements of H with CO and CB states are equal. Let

$$(\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n) = E(\mathbf{p}_1 \cdots \mathbf{h}_n) \ , \tag{3.14}$$

we have

$$\langle \mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n \rangle - E = \langle \mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H - E \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n \rangle \ , \tag{3.15}$$

and

$$\{\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H - E \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n\} = 0 + \text{terms of order } 1/\Omega \ . \tag{3.16}$$

From the definition of CO state (3.2) and Eq. (3.16) we obtain

$$\langle \mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H - E \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n \rangle = x_2 + x_3 + \cdots \ , \tag{3.17}$$

where x_i are sums of products of i nondiagonal matrix elements. The x_2 is given by

$$x_2 = x_{2,1} + x_{2,2} \ , \tag{3.18}$$

$$x_{2,1} = -\tfrac{1}{2} \sum_{\mathbf{p}' \cdots \mathbf{h}'_n} \overline{\{\mathbf{p}_1 \cdots \mathbf{h}_n \,|\, H - E \,|\, \mathbf{p}'_1 \cdots \mathbf{h}'_n\}} \times \overline{\{\mathbf{p}'_1 \cdots \mathbf{h}'_n \,|\, \mathbf{p}_1 \cdots \mathbf{h}_n\}} + \text{c.c.} \ , \tag{3.19}$$

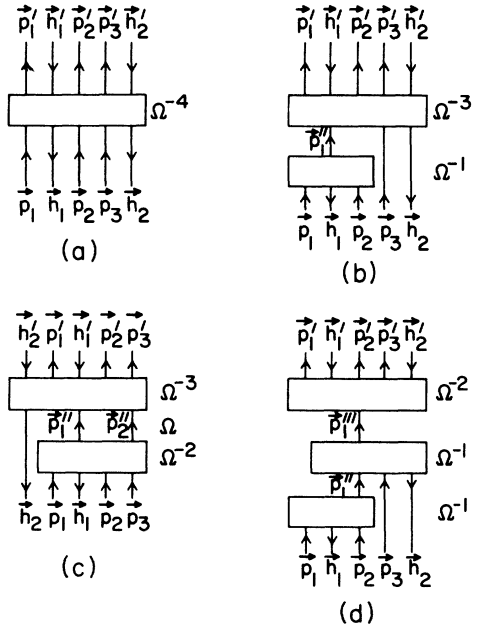

FIG. 6. Diagrams representing terms in $\{\mathbf{p}_1'\cdots\mathbf{h}_n' \mid \mathbf{p}_1\cdots\mathbf{h}_n\}$.

$$x_{2,2}=\tfrac{1}{4}\sum_{\mathbf{p}_1'\cdots\mathbf{h}_n'} \overline{|\{\mathbf{p}_1\cdots\mathbf{h}_n \mid \mathbf{p}_1'\cdots\mathbf{h}_n'\}|^2} \times\{\mathbf{p}_1'\cdots\mathbf{h}_n' \mid H-E \mid \mathbf{p}_1'\cdots\mathbf{h}_n'\} , \quad (3.20)$$

and if $|\mathbf{p}_1\cdots\mathbf{h}_n\}$ differs from $|\mathbf{p}_1'\cdots\mathbf{h}_n'\}$ in D states the order of magnitude of x_2 is $\Omega^{-D+S}\leq\Omega^{-1}$. In a similar way we can show that all the x_i $(i\geq 2)$ are of order of magnitude $\leq\Omega^{-1}$, and hence we obtain the desired result.

$$\langle\mathbf{p}_1\cdots\mathbf{h}_n \mid H \mid \mathbf{p}_1\cdots\mathbf{h}_n\rangle=(\mathbf{p}_1\cdots\mathbf{h}_n \mid H \mid \mathbf{p}_1\cdots\mathbf{h}_n) + \text{terms of order } 1/\Omega . \quad (3.21)$$

A similar procedure has been used[20] to orthogonalize the states of few-body systems. The states are classified according to the number of particles in the continuum. The states $|0,I)$, for example, denote all the bound states, while $|1,I)$ denote states where one particle is in unbound continuum, and the rest are bound, etc. The energies of these states are known from the spectra of the bound system, and a way to obtain orthonormal states with the correct energies is to Schmidt orthogonalize the states $|n,I)$ to all states $|m<n,J)$ to obtain PO states $|n,I\}$, and then use the Löwdin transformations to orthogonalize them.

IV. COMPARISON OF OCB WITH CBF THEORY

Orthogonal and nonorthogonal CB theories make use, in general, of different perturbative schemes to calculate various quantities of interest. In OCB theory the basis states are properly orthogonalized; therefore, standard perturbative techniques are adopted and the corresponding schemes at each perturbative order do not contain any spuriosity concerned with orthogonalization. On the contrary, in CBF theories, every order of the perturbative series contains spurious terms, and the due orthogonality corrections come only from higher order contributions.

In this section we discuss the nature and the implications of such orthogonality corrections which, in most of the CBF calculations performed until now, have been neglected. To this aim, we analyze the calculations of the dynamical structure function[16] and of the nondiagonal matrix elements of the Hamiltonian between states having two different orbitals. These matrix elements enter into the calculation of the perturbative corrections to the ground state energy,[9,12] the optical potential,[12] as well as that of the particle-hole effective interaction. We will limit our analysis to the first order terms in the power series (PS) expansion,[19] namely those having only one dynamical correlation amongst the particles which are not directly connected by the Hamiltonian operator.

For the sake of simplicity, we consider the case of a correlation operator of the Jastrow type, but similar arguments and conclusions can be drawn for the more general case of a state dependent correlation operator.

A. Dynamical structure function

A dynamical structure function $S(\mathbf{k},\omega)$ is obtained from the density-density correlation function

$$S(\mathbf{k},\omega)=\frac{1}{\pi}\,\mathrm{Im}D(\mathbf{k},\omega) , \quad (4.1)$$

$$D(\mathbf{k},\omega)=\langle\bar{0} \mid \rho_{\mathbf{k}}^{\dagger}(H-\bar{E}_0-\omega-i\eta)^{-1}\rho_{\mathbf{k}} \mid \bar{0}\rangle , \quad (4.2)$$

$$\rho_{\mathbf{k}}=\sum_{i=1,A}\exp(i\mathbf{k}\cdot\mathbf{r}_i) , \quad (4.3)$$

where $|\bar{0}\rangle$ is the exact ground state with energy $\bar{E}_0$. Formally, the Hamiltonian H is written as a sum of an unperturbed part H_0 and an interaction term H_I defined by the following equations:

$$\langle m \mid H_0 \mid n\rangle=(m \mid H \mid m)\delta_{mn} , \quad (4.4)$$

$$\langle m \mid H_I \mid n\rangle=\langle m \mid H \mid n\rangle(1-\delta_{mn}) , \quad (4.5)$$

and the right-hand side (rhs) of Eq. (4.2) is expanded around $H_I=0$. For the present purposes it suffices to keep only the very first term of the expansion, which is equivalent to say that, in Eq. (4.2), we approximate H with H_0 and assume the CB state $|0)$ to be the exact ground state $|0\rangle$ and consider the 1p-1h CO states as the only intermediate states. Under these assumptions $S(\mathbf{k},\omega)$ is given by

$$S_{ph}^{(0)}(\mathbf{k},\omega)=\sum_{h_i}|X(\mathbf{p}_i\mathbf{h}_i)|^2\delta[e(p_i)-e(h_i)-\omega] , \quad (4.6)$$

$$X(\mathbf{p}_i\mathbf{h}_i)=\langle\mathbf{p}_i\mathbf{h}_i \mid \rho_{\mathbf{k}} \mid 0\rangle , \quad (4.7)$$

where $e(p_i)$ and $e(h_i)$ are single particle energies,[12] and $\mathbf{p}_i=\mathbf{h}_i+\mathbf{k}$.

The OCB state $|p_ih_i\rangle$ is given by

$$|\mathbf{p}_i\mathbf{h}_i\rangle = |\mathbf{p}_i\mathbf{h}_i) - \tfrac{1}{2}\sum_j |\mathbf{p}_j\mathbf{h}_j)\overline{(\mathbf{p}_j\mathbf{h}_j|\mathbf{p}_i\mathbf{h}_i)} + \cdots , \quad (4.8)$$

since the PO 1-ph states $|p_ih_i\} = |p_ih_i)$. The $X(p_ih_i)$ can be calculated as

$$\xi(i) \equiv (\mathbf{p}_i\mathbf{h}_i|\rho_{\mathbf{k}}|0) , \quad (4.9)$$

$$N(ij) = (\mathbf{p}_i\mathbf{h}_i|\mathbf{p}_j\mathbf{h}_j)(1-\delta_{ij}) , \quad (4.10)$$

$$X(\mathbf{p}_i\mathbf{h}_i) = \xi(i) - \tfrac{1}{2}\sum_j N(ij)\xi(j) + \tfrac{3}{8}\sum_{j,l} N(ij)N(jl)\xi(l) + \cdots . \quad (4.11)$$

In nonorthogonal CBF theory $X(\mathbf{p}_i\mathbf{h}_i)$ is approximated with $\xi(i)$; the higher terms in Eq. (4.11) are orthogonality corrections. Both $\xi(i)$ and $N(ij)$ have a diagramatic expansion given in Ref. 16. It is interesting to analyze the cancellations among the various terms in $X(p_ih_i)$, they reveal the spurious contributions in $\xi(i)$.

The zeroth and first order terms of $\xi(i)$ are given by[16]

$$\xi(i) = \xi^{(0)}(i) + \xi^{(1)}(i) + \cdots , \quad (4.12)$$

$$\xi^{(0)}(i) = D(7,1) , \quad (4.13)$$

$$\xi^{(1)}(i) = D(7,2) + D(7,3) + \tfrac{1}{2}D(7,4) + \tfrac{1}{2}D(7,5) + D(7,6) , \quad (4.14)$$

where $D(7,i)$ are diagrams of i of Fig. 7. $N(ij)$ has no zeroth order contribution, and in first order it is given by

$$N^{(1)}(ij) = D(7,7) + D(7,8) . \quad (4.15)$$

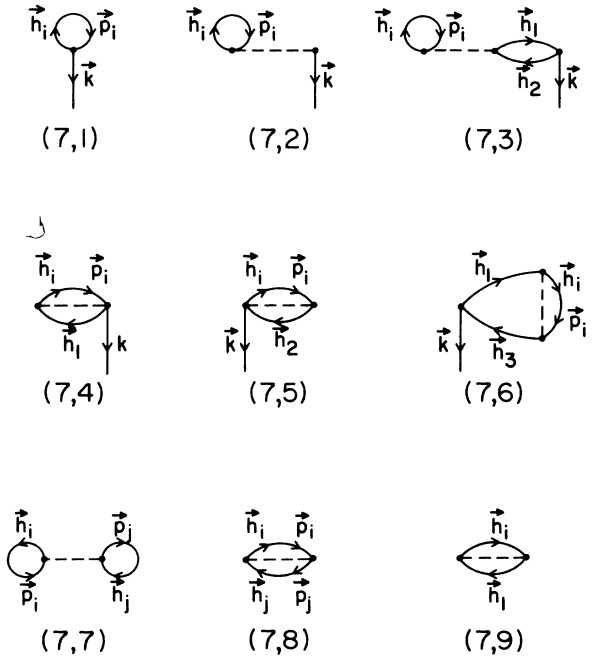

FIG. 7. The zeroth order contribution to $\xi(i)$ is given by 7,1. First order diagrams 7,2-7,6 contribute to $\xi(i)$; 7,7 and 7,8 contribute to $(\mathbf{p}_i\mathbf{h}_i|\mathbf{p}_j\mathbf{h}_j)$, and 7,9 to vertex correction $X_{\text{c.c.}}(h_i)$. A sum over $\mathbf{h}_1, \mathbf{h}_2$, and $\mathbf{h}_3$ is implied.

In order to calculate $X(\mathbf{p}_i\mathbf{h}_i)$ up to first order we need to consider only the term $\frac{1}{2}N^{(1)}(ij)\xi^{(0)}(j)$ from orthogonality corrections. It is easy to multiply diagrams and sum over j as illustrated in Fig. 8. The product of the zeroth order ξ diagram (7,1) with the first order N diagrams (7,7) and (7,8) gives the four diagrams (7,2), (7,3), (7,4), and (7,6). It follows that $X(p_ih_i)$ differs from $\xi(i)$ due to orthogonality corrections: in fact, diagram (7,4) is completely cancelled and the remaining first order diagrams come all with a factor $\frac{1}{2}$:

$$X^{(0)}(p_ih_i) = \xi^{(0)}(i) , \quad (4.16)$$

$$X^{(1)}(p_ih_i) = \tfrac{1}{2}[D(7,2) + D(7,3) + D(7,5) + D(7,6)] , \quad (4.17)$$

It is worth mentioning that diagram (7,4), if included in $X(\mathbf{p}_i\mathbf{h}_i)$, would lead to a violation of the sum rule

$$\frac{1}{A}(0|\rho_{\mathbf{k}}^{\dagger}\rho_{\mathbf{k}}|0) = S(k) = \int d\omega\, S_{ph}(k,\omega) = \sum_{\mathbf{h}_i} |X(\mathbf{p}_i\mathbf{h}_i)|^2 . \quad (4.18)$$

The last equality holds on account of the fact that the density fluctuation operator $\rho_{\mathbf{k}}$ commutes with the Jastrow correlation operator and, therefore, $\rho_{\mathbf{k}}|0\rangle$ is a combination of 1p-1h CO states. It is easy to verify that diagram (7,4) can be folded into a part which coincides with diagram (7,1) and a vertex correction[7] $\tilde{X}_{\text{c.c.}}(h_i)$ given by diagram (7,9) depending on the hole momentum h_i only. As a consequence, when it is included in $X(\mathbf{p}_i\mathbf{h}_i)$ appearing in Eq. (4.18), it generates terms which are independent of k and, therefore, violate the property of $S(k)$ to heal to one when k goes to infinity. Similar cancellations of diagrams are also present at higher orders of the PS expansion and a cluster decomposition of $X(\mathbf{p}_i\mathbf{h}_i)$ at all the orders is not known yet. However, Eq. (4.11) can be numerically solved by means of an iterative procedure,[16] few iterations being sufficient to reach the convergence.

In absence of correlations $\xi = X = 1$. Thus, the quantity $1-X$ measures the effect of correlations, and in

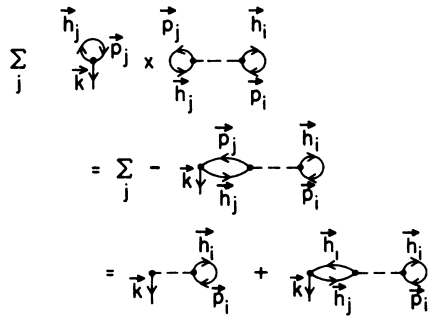

FIG. 8. Illustration of diagrammatic multiplication. The second equality is obtained by writing the sum over $\mathbf{p}_j$ as a sum over all states minus the sum over hole states. Sum over $\mathbf{h}_1$ is implied as in Fig. 7.

TABLE I. Typical values of the quantities $1-\xi$ and $1-X$ for a Jastrow model of nuclear matter at $k_F=1.33$ fm^{-1}. ξ and X are given for $h=0.56$ fm^{-1} and $p=k$. The pair correlation and the Fermi-hypernetted chain (FHNC) equations given in Ref. 16 are used to obtain these results.

k/k_F	1	1.5	2	2.5
$1-\xi$	0.14	0.14	0.10	0.06
$1-X$	0.07	0.08	0.06	0.04

nonorthogonal theories it is approximated by $1-\xi$. We see from Table I that $1-\xi$ is much larger than $1-X$ showing that it is necessary to treat orthogonality corrections to calculate correlation effects in $S(k,\omega)$.

B. Correlation energy

The second order perturbative correction to the ground state energy E_0 is given by

$$\Delta E_0^{(2)}=\tfrac{1}{4}\sum_{\mathbf{p}_1,\mathbf{p}_2,\mathbf{h}_1,\mathbf{h}_2}\frac{|\,H(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\,|^2}{e(h_i)+e(h_j)-e(p_i)-e(p_j)}\,, \tag{4.19}$$

$$H(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)=\langle 0\,|\,H\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j\rangle\,. \tag{4.20}$$

In nonorthogonal CBF theory the matrix element $H(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)$ has the following expression:

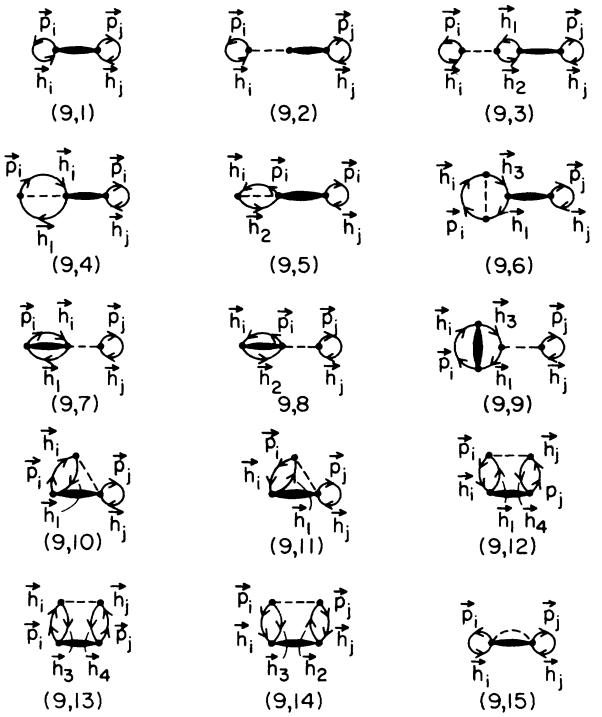

FIG. 9. Diagrams 9,1-9,14 give the zeroth and first order contributions to $H_{\rm CBF}(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)$. First order orthogonality corrections change the contributions of Diagrams 9,2-9,7 and 9,9-9,14, and give the new diagram 9,15.

$$\begin{aligned}H_{\rm CBF}(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)&=(0\,|\,H-E_0\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\\&=(0\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\left[\frac{\hbar^2}{2m}(p_i^2+p_j^2-h_i^2-h_j^2)-\Sigma_c(I+\mathbf{h}_i)-\Sigma_c(I+\mathbf{h}_j)\right]\\&\quad+\Sigma_1(\mathbf{p}_i\mathbf{h}_i+\mathbf{p}_j\mathbf{h}_j+\text{connected }I)\Big/\left\{\left[1+\Sigma_c(p_i)\right]\left[1+\Sigma_c(p_j)\right]\left[1+\Sigma_c(h_i)\right]\left[1+\Sigma_c(h_j)\right]\right\}^{1/2}\end{aligned} \tag{4.21}$$

The $(0\,|\,\mathbf{p}_1\mathbf{p}_2\mathbf{h}_1\mathbf{h}_2)$ has no zeroth order contribution. In first order it is given by diagrams (7,7) and (7,8) on replacing the transition line $\mathbf{h}_i\mathbf{p}_i$ with $\mathbf{p}_i\mathbf{h}_i$. The second term of (4.21) has zeroth and first order contributions illustrated by diagrams (9,1)–(9,14) of Fig. 9. These are denoted by $D(9,k=1,14)$. The remaining direct diagrams contributing to the second term are obtained by interchanging $\mathbf{p}_i\mathbf{h}_i$ with $\mathbf{p}_j\mathbf{h}_j$ in diagrams (9,2)–(9,12). These diagrams are denoted by $DS(9,k=2,12)$. There are no $DS(9,k=1$ or $13,14)$ diagrams because $D(9,k=1$ or $13,14)$ are symmetric under this interchange. Exchange diagrams $DE(9,k=1,14)$ and $DSE(9,k=2,12)$ are obtained by exchanging $\mathbf{h}_i$ with $\mathbf{h}_j$. We obtain

$$\begin{aligned}H_{\rm CBF}(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)&=T_1+\sum_{k=1,14}[D(9,k)+DE(9,k)][1-\tfrac{1}{2}\delta_{k4}-\tfrac{1}{2}\delta_{k5}]\\&\quad+\sum_{k=2,12}[DS(9,k)+DSE(9,k)][1-\tfrac{1}{2}\delta_{k4}-\tfrac{1}{2}\delta_{k5}]\,,\end{aligned} \tag{4.22}$$

where T_1 is the first term in Eq. (4.21). Note that there is partial cancellation of diagrams having $k=8$ with the terms in T_1.

In OCB theory the PO states $|\,\mathbf{p}_i\mathbf{h}_j\mathbf{h}_i\mathbf{h}_j\}$ with zero total momentum are given by

$$|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j\}=|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)-|\,0)(0\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\,, \tag{4.23}$$

since $(\mathbf{p}_1\mathbf{h}_1\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)=0$ for such states. Thus

$$\{0\,|\,H\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j\}=(0\,|\,H-E_0\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\,, \tag{4.24}$$

and the CBF theory takes into account the nonorthogonality of the ground and $|\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)$ states. In order to analyze the effect of the nonorthogonality of states $|\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)$ and $|\mathbf{p}'_i\mathbf{p}'_j\mathbf{h}'_i\mathbf{h}'_j)$, etc., we calculate the first order Löwdin correction to this matrix element:

$$\Delta H(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)=-\tfrac{1}{2}\sum_{2'}(0\,|\,H-E_0\,|\,2')(2'\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\ , \tag{4.25}$$

where the 2p-2h states $|\,2')$ have two momenta different from $\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j$, namely

$$|\,2')\ni|\,\mathbf{p}'_i\mathbf{p}_j\mathbf{h}'_i\mathbf{h}_j),\ |\,\mathbf{p}'_i\mathbf{p}'_j\mathbf{h}_i\mathbf{h}_j),\ |\,\mathbf{p}'_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}'_j),\ |\,\mathbf{p}_i\mathbf{p}'_j\mathbf{h}_i\mathbf{h}'_j),\ |\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}'_i\mathbf{h}'_j),\ |\,\mathbf{p}_i\mathbf{p}'_j\mathbf{h}'_i\mathbf{h}_j)\ . \tag{4.26}$$

States having three or four momenta $\mathbf{p}'_i\mathbf{p}'_j\mathbf{h}'_i\mathbf{h}'_j$ different from $\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j$ do not contribute to ΔH in the first order of PS expansion.

The products of zeroth order terms of $(0\,|\,H-E_0\,|\,2')$ (i.e., those without a dashed line) with the first order terms of $(2'\,|\,\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)$ also generate all the first order diagrams of Fig. 9. Thus up to first order terms we get

$$\begin{aligned}H_{\rm OCB}(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)&=H_{\rm CBF}(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)+\Delta H(0;\mathbf{p}_i\mathbf{p}_j\mathbf{h}_i\mathbf{h}_j)\\&=T_1+D(9,1)+DE(9,1)+\sum_{k=2,14}\tfrac{1}{2}[D(9,k)+DE(9,k)][1-\delta_{k5}+\delta_{k8}]\\&\quad+\sum_{k=2,12}\tfrac{1}{2}[DS(9,k)+DSE(9,k)][1-\delta_{k5}+\delta_{k8}]-\tfrac{1}{2}[D(9,15)+DE(9,15)]\ .\end{aligned} \tag{4.27}$$

We note that the orthogonality corrections completely cancel the diagram $D(9,5)$ along with its *DS*, *DE*, and *DSE* counterparts, and they reduce the contribution of all other first order diagrams except $D(9,8)$ and its counterparts, by a factor of 2. However, new diagrams $D(9,15)$ and $DE(9,15)$ are added. Thus, it is not consistent to calculate the first order PS corrections to the matrix element without taking into account the orthogonality corrections. Particularly, in dense systems like ^{3}He diagrams of type $D(9,5)$ give large contributions[9] in nonorthogonal theories, and these may be entirely spurious.

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